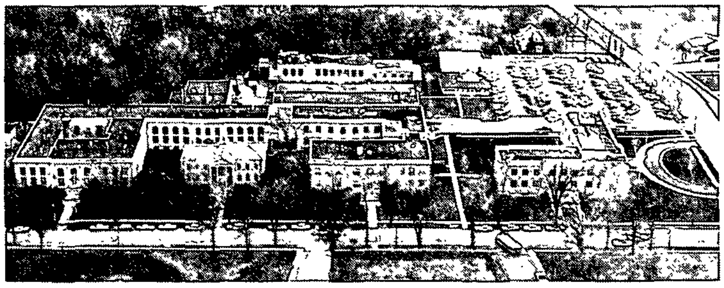

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OPTIMIZATION AND FLOW SHEET SIMULATION

P. E. PARKER, K. E. SAFFRAN, AND F. W. AHRENS

USE OF A NEW PULP AND PAPER SYSTEM SIMULATION PROGRAM FOR KRAFT PULP MILL OPTIMIZATION

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OPTIMIZATION AND FLOW SHEET SIMULATION

by

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ABSTRACT

Recent work by Biegler (8) has investigated optimization techniques for sequential, modular flow sheet simulators. This work extends that effort. Successive linear programming coupled with a reduced gradient method gave fast, reliable optimization. A kraft pulping process involving 22 modules and 50 streams was optimized. Compared to the base case, significantly improved operating points were located.

INTRODUCTION

Environmental restrictions, the cost of capital, and a host of other factors are tending to reduce profit margins for pulp and paper mills. Simulation is gaining recognition as a tool that can help mills improve profitability through computer aided studies of process alternatives, as parts of mill-wide control systems, and through its role in optimization.

Sequential, modular simulation programs are probably the most widely used steady-state simulators in the pulp and paper industry. Their method of solution does not readily lend itself to process optimization, as constraints on processing conditions or stream flows are not easily implemented. Recent work at The Institute of Paper Chemistry has explored various ways of coupling optimization programs with a sequential modular simulator. This work has shown that proven optimization methods (successive linear programming and the reduced gradient method) can be easily coupled to a simulator to give a powerful, robust tool.

Steady-state, sequential, modular simulators embody three major characteristics as exemplified by their name. The processes to be modelled are assumed to be at steady state. While this is never true for any real process, long-term averages can be assumed to represent an average steady state. Similarly, various short-term operations can also be assumed to be at steady state. Finally, steady-state simulation can give the goals for a process control system. The variances inherent in a control scheme are departures from the ideal state.

The modular nature of the simulation programs implies that the process is built from a library of pre-existing process models. The user usually has no information on the exact equations used in the model, the computer variable names, or the order in which equations are set up and solved by the model. The user supplies parameters that represent operating conditions or coefficients for correlations, and the model converts input flows to output flows. The simulator computes material and energy balances by solving the appropriate balance equations for each module in a specified sequence. Usually the user specifies the sequence of calculations, but it may be determined by the simulator. The attributes of recycle streams must be estimated by the user, and the simulator improves the estimate by repeating the calculation sequence many times and continually improving the estimates of the tear streams. At no time does the simulator work with more than the streams connected to a single process model and the balance equations for that model (i.e., the solution method is sequential).

These are critical points when considering coupling an optimization program to a sequential, modular simulator.

OPTIMIZATION

From a mill operations point of view, optimization is the process of finding an operating point that maximizes the marginal return on investment, given constraints on raw material supply, availability of capital, and operability of the process. In a general sense, the optimization problem can be stated as:

$$\min f(X);\ X = x_1, x_2, \ldots x_n \tag{1}$$

$$g_j(X) > 0;\ j = 1,2, \ldots p \tag{2}$$

$$h_k(X) = 0;\ k = 1,2, \ldots q \tag{3}$$

where X is the vector of design variables. An allowed range on any variable is easily converted into two inequality constraints and becomes part of the set of constraints g_j and h_k.

It is possible to maximize f(X) by minimizing -f(X). In this discussion we will consider the minimization problem, even though the actual marginal return on investment problem should be maximized. This is easily done by changing the sign on the objective function, f(X).

Many methods exist for attacking this nonlinear constrained optimization problem. The earliest methods recast the problem into an unconstrained problem and then used the wealth of methods available for the unconstrained problem. The simplest method of reformulating the constrained problem is the penalty function method. In this approach, the cost associated with violating the constraints is made a dominant factor in the problem. Thus, optimization methods are forced to stay within the hypervolume defined by the constraints. Another method is to modify the random search procedure to discard points that violate the constraints. The complex method of Box (1) can work directly with the constrained problem. Regions of active constraints cause the complex to shrink, while areas with few or no constraints cause the complex to expand and thus move rapidly to a local optimum.

It is well known that if the problem (the objective function and its constraints) are linear, then linear programming can quickly find the optimal solution. The method of successive linear programming, devised by Griffith and Stewart (2), converts the nonlinear problem to a linear problem and solves the linear approximation. The problem is converted to:

$$f(X^{t+1}) - f(X^t) = \sum \frac{\partial f}{\partial x_i} \Delta x_i \tag{4}$$

$$\sum_{i=1}^{n} \frac{\partial g_j}{\partial x_i} \Delta x_i - g_j(x^t) \geq 0; \; j = 1 \ldots p \tag{5}$$

$$\sum_{i=1}^{n} \frac{\partial h_k}{\partial x_i} \Delta x_i = 0; \; k = 1 \ldots q \tag{6}$$

This linearized problem is solved by an LP routine which returns a displacement ΔX. A new solution point is then found by incrementing the current value of X by the displacement:

$$X^{t+1} = X^t + \Delta X \tag{7}$$

The problem is linearized about the new estimate, X^{t+1}, and the process is repeated. Usually a limit is placed on the allowable displacement, ΔX, to ensure that the linearization remains a good approximation.

Constrained optimization problems can be solved directly, but with more effort than that required for the unconstrained case. The reduced gradient method and the method of successive quadratic programming are two popular methods. The reduced gradient method can only work with equality constraints. Fortunately, this poses no severe limitation, since inequality constraints can be converted to equality constraints through the use of slack variables. The slack variables become independent variables in the problem, thus effectively increasing the dimension of the problem. The procedure is to divide the independent variables into two sets: a basic set and a nonbasic set. In essence, the objective function is optimized in the nonbasic variables while adjusting the basic variables to maintain the solution within the feasible space. If during the search, one of the variables in the basic set must move beyond its upper or lower bound, then that variable is swapped with a variable in the nonbasic set. This procedure is well defined by Wolfe (3) and Abadie and Carpentier (4).

The method of Successive Quadratic Programming involves approximating the objective function with a second order Taylor series:

$$f(X + \Delta X) = f(X) + \nabla f(X)\ \Delta X + 1/2\ \Delta X\ \nabla^2 f(X) \Delta X \tag{8}$$

The function

$$f(X + \Delta X) - f(X) \tag{8a}$$

or, equivalently,

$$\nabla f(X)\ \Delta X + 1/2\ \Delta X\ \nabla^2 f(X) \Delta X \tag{8b}$$

is minimized subject to:

$$g_j\ (X) + \nabla g(X)\ \Delta X \geq 0;\ j = 1 \ldots p \tag{9}$$

$$h_k\ (X) + \nabla h(X)\ \Delta X = 0;\ k = 1 \ldots q \tag{10}$$

This is a quadratic programming problem and can be solved by such routines. The major drawback is the formulation and/or calculation of the Hessian. Han (5) and Powell (6) have recently suggested a modification to the method that introduces second order Lagrangian constraint information and have suggested using the Broyden-Fletcher-Goldfarb-Shanno (BFGS) approximation to the Hessian. These modifications have made the method very powerful, but difficulties have been experienced in applying them (7,8).

SIMULATION/OPTIMIZATION

In principle, any of the optimization methods can be intimately coupled with a simulation program to provide a simulation and optimization capability in one package. The major task is to isolate the various independent and dependent variables. Constraints become one of two types: external and internal. External constraints are supplied by the user. Internal constraints are supplied by the simulator, the models within the simulator, and the interrelations contained in the flow sheet to be simulated. The simulator also supplies the functional relationship among the variables and, thus, the necessary partial derivatives for the Jacobian or Hessian must be evaluated numerically. Since converged simulations are needed to evaluate the Jacobian and/or Hessian, a premium is placed on minimizing the number of times these matrices must be updated. Obviously, methods such as the BFGS update procedures must be utilized in the optimization scheme.

Loose coupling of an optimization routine to a flow sheet package can occur in one of three ways, as illustrated in Figure 1. The Direct Link Interface, or DLI, makes the simulator a simple subset of the optimization procedure. Whenever functions need to be evaluated, the optimization package calls the simulator to develop a converged simulation. The major problem is to develop a simple scheme for the simulator and the optimization package to communicate data needs and results.

The Approximation Interface (AI) does not allow the optimization program to communicate directly with the process simulator. The AI uses the simulator to

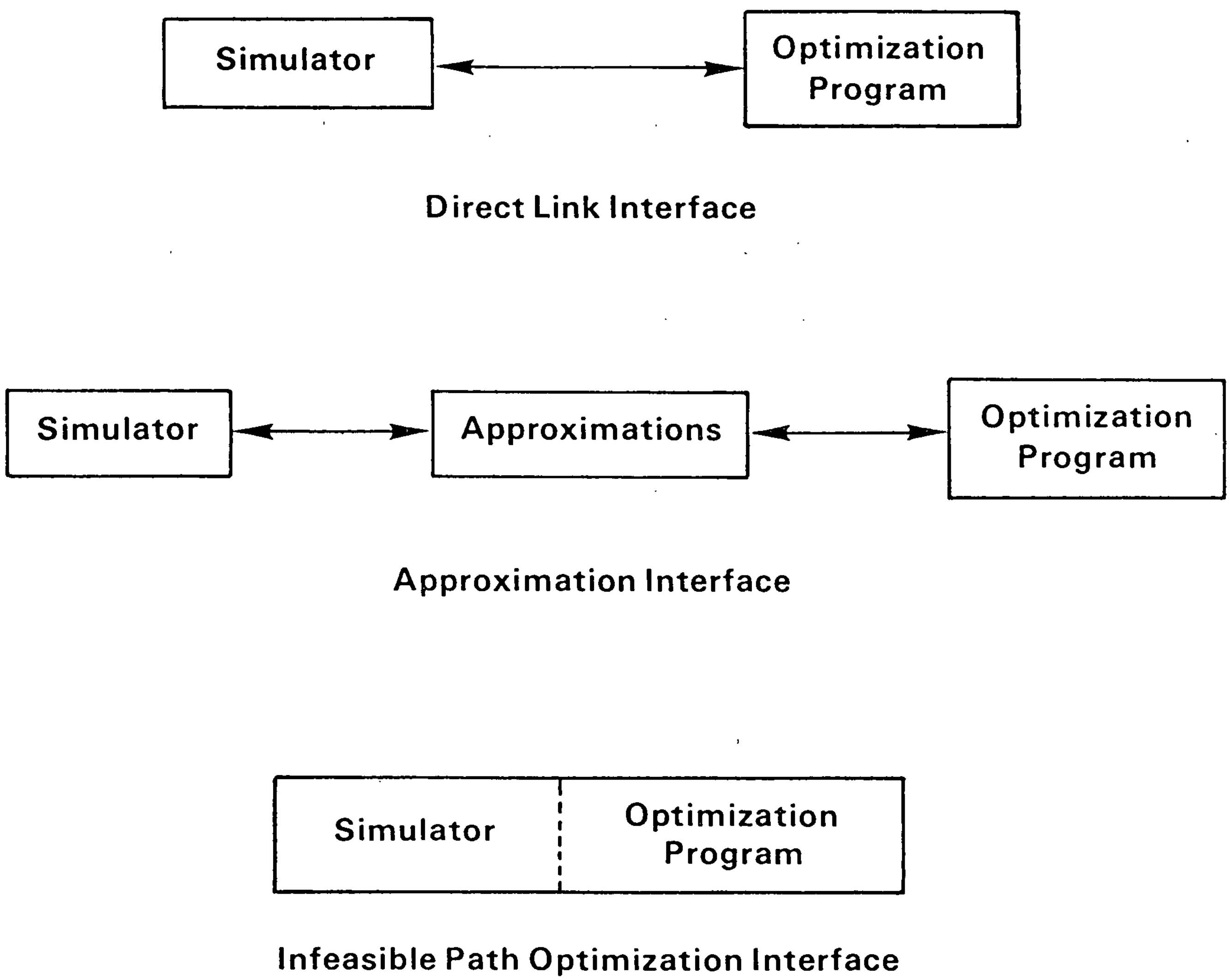

Figure 1. Schematics of the three interface formats.

develop the data necessary to develop linear or quadratic approximations of the objective function and constraints in terms of the independent variables. The optimization program then uses these approximations for its function evaluations. The two-step procedure of approximation and optimization is repeated until a solution is found.

The third type of interface is the complete integration of the simulator and optimization packages. Such integration requires recoding of the simulator/optimizer interface whenever a new optimization method is desired. This type of integration, however, allows the entire problem--convergence and optimization--to be solved in one pass. That is, the only solution is a converged solution at an optimum. An example of this method is the Infeasible Path Optimization method, proposed by Beigler (8). The IPO method effectively adds all the components of the tear streams to the optimization problem as independent variables. For all problems tested in this work, the IPO method was found to be very unsatisfactory and noncompetitive with either the DLI or AI type methods. Further investigation of a totally integrated package was halted to pursue study of the DLI and AI methods.

THE SIMULATOR

MAPPS, Modular Analysis of Pulp and Paper Systems (9), was chosen as the simulator for this study. MAPPS contains approximately 60 process models ranging from simple splitters and mixers to complex digester models. MAPPS, as its name indicates, is designed primarily for the pulp and paper industry. The modules allow virtually all processes in an integrated unbleached kraft mill to be simulated; bleach plant models are under development by The Institute of Paper Chemistry and will be available in the near future.

THE TEST PROBLEM

Several pulping and recovery problems were used to test various optimization methods and the two interfaces. One of these problems, the kraft pulping study utilizing batch digesters, will be discussed here. Discussions of the other problems, and of the difficulties in use of the IPO method, can be found in (10).

The flow sheet for this conventional kraft pulping process is shown in Figure 2. The process modules are defined in Table 1, and the attributes of the streams are given in Table 2. Note that the pulping streams contain 19 chemical species as well as temperature, pressure, and enthalpy.

The test case was to minimize the hourly operating costs by manipulating the eight independent variables given in Table 3. The costs include charges for wood, lime, hydroxide, and fuel oil for the kiln and boilers. Credit was given for electricity produced. No credit was taken for the pulp produced, as pulp production was held constant, as shown in the list of constraints in Table 4.

These constraints make for a realistic problem. The production constraint is equivalent to 1000 tpd of bone dry pulp. The digester downtime constraint forces the optimizer to consider some production loss due to filling and blowing the digesters. If this constraint were removed, the process would be driven to a zero downtime, thus simulating a continuous digester. The restrictions on heating time and liquor:wood ratio ensure reasonable simulations. The H-factor constraint is used as a quality control restriction.

Several optimization methods, listed in Table 5, were used with the DLI and AI to solve this problem. Three of the methods, GS, OPT, and VF02AD found essentially the same solution, given in Table 6. BIAS and SEEK made no significant progress on the problem. This, and other test problems, showed that GS

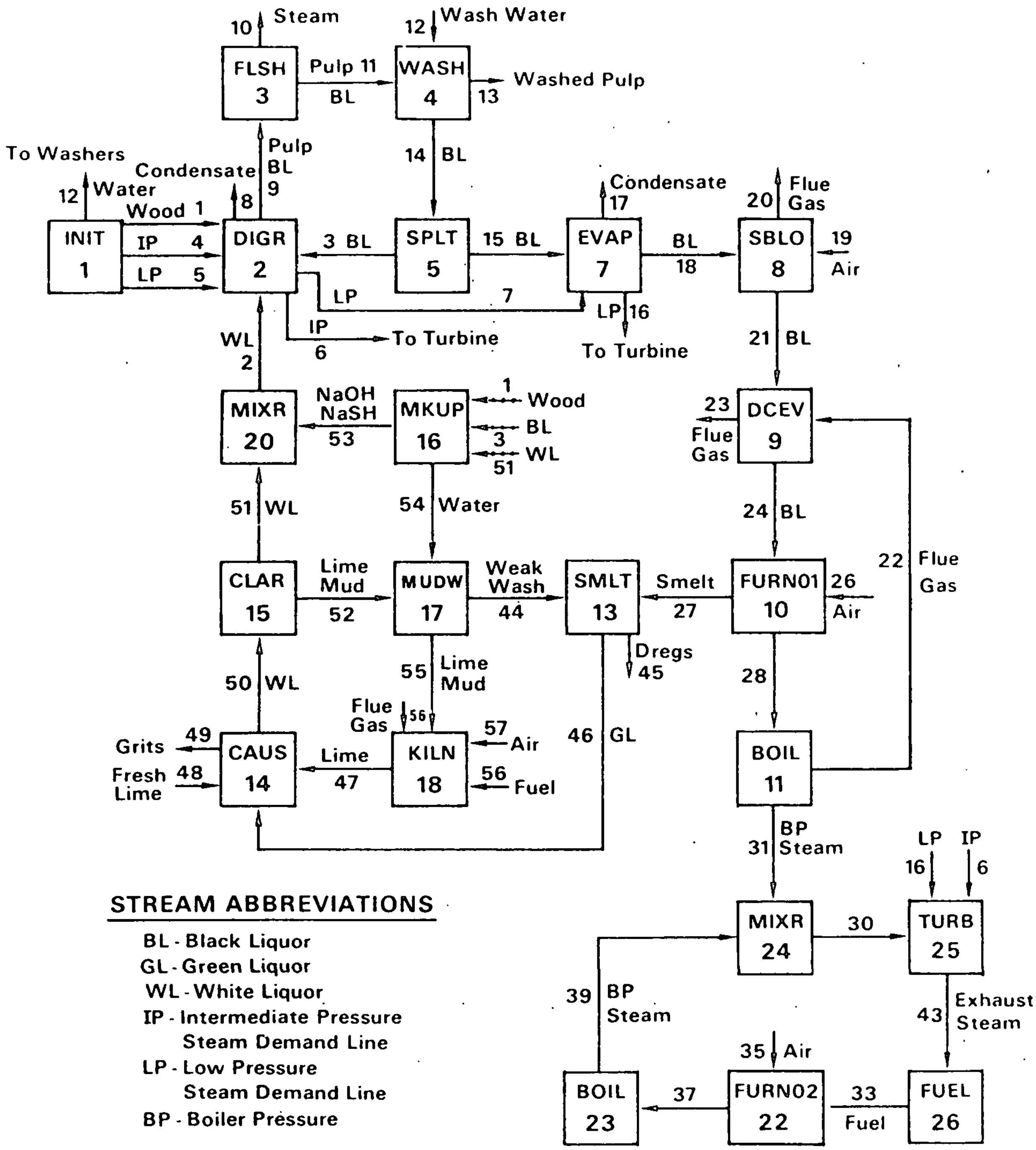

Figure 2. MAPPS diagram for pulping problem.

Table 1. Descriptions of the modules used in the pulping problem.

Module	Description
BOIL	A steam generation unit for a recovery or power boiler.
CAUS	A causticizing and slaking module. The causticizing efficiency is specified.
CLAR	A white liquor clarifier module.
DCEV	A direct contact evaporator model. The product liquor concentration is calculated based on the inlet conditions of the flue gas and liquor, and on the specified difference between the outlet flue gas and liquor temperatures.
DIGR	A batch digester module. The yield, kappa number, pulp viscosity and residual pulping chemicals are calculated using regression equations developed by Dr. Tom McDonough at IPC.
EVAP	A multiple effect evaporator module which calculates the product liquor concentration and steam economy using specified values for the average heat transfer rate and the number of effects.
FLSH	A flash tank.
FUEL	A fuel controller that regulated the amount of fuel used by the power boiler in order to force the turbine exhaust steam flow to zero.
FURN01	A recovery furnace combustion unit. The reduction ratio is specified.
FURN02	A power boiler combustion unit.
INIT	An initialization module that sets the wood flow, washer shower flow, and the base steam demands.
KILN	A rotary lime kiln module.
MIXR	A stream mixer.
MKUP	A makeup controller. It controlled the water flow to the mud washer, NaOH flow, and NaSH flow to meet active alkali concentration, active alkali charge, and sulfidity specifications.
MUDW	A mud washer module.
SBLO	A strong black liquor oxidation module.
SMLT	A smelt dissolving tank.
SPLT	A flow splitter.
TURB	A three stage steam turbine. The amount of electricity generated is based on the amount of boiler steam available and on the mill steam demands.
WASH	This module simulates a set of countercurrent vacuum drum washers. The model is taken from Perkins, et al.

Table 2. List of components for the pulp and liquor streams in the pulping problem.

Temperature	Sodium Na^+
Pressure	Organic Ion
Heat Capacity	Hydroxide OH^-
Enthalpy	Hydrosulfide SH^-
Total Flow	Sulfide S^{-2}
Water	Thiosulfate $S_2O_3^{-2}$
Cellulose	Sulfate SO_4^{-2}
Lignin	Carbonate CO_3^{-2}
Dissolved Cellulose	Chlorine Cl^-
Dissolved Lignin	$CaCO_3$
Bound Sodium	CaO
Bound Organics	CaO Inert

Table 3. Descriptions of pulping problem.

Objective: Minimize the net variable cost, including wood, chemical, and fuel costs, and a credit for power produced

Independent Variables:

	Starting Value	Range
Cooking time, fraction of total cycle time (hours)	0.5 (2.0)	0-1.0
Heating time, fraction of total cycle time (hours)	0.375 (1.5)	0-1.0
Cooking temperature, °F	340	320-360
Active alkali charge, in Na_2O on wood	18%	16-20%
Sulfidity, %	25%	20-30%
Active alkali concentration in white liquor, lb/ft	6.0	5.8-6.2
Black liquor recycle split, fraction to digester	0.3	0.1-0.5
Wood flow, wet, 50% moisture, lb/hr	376,930	300,000-400,000

Table 4. Pulping problem constraints.

Contraints:

	Subproblem T2B
Pulp production, lb/hr	$\frac{\text{Pulp}-83340}{83340} = 0$
H-Factor[a]	$\frac{\text{HF}-2237}{2237} = 0$
Furnace liquor solids concentration	Conc.-0.6496 = 0
Digester downtime, hr	0.49-20
Heating + cooking time fractions Heating time, hr	1.0-10
Liquor-to-wood ratio*	3.5-4.0

*Defined as weight of total liquor to weight of dry wood.

Table 5. Description of optimization programs evaluated.

Program Name	Description	Source
BIAS	Davidon-Fletcher-Powell unconstrained search with method of multipliers penalty function	School of Mechanical Engineering, Purdue University[a]
OPT	Reduced gradient search	School of Mechanical Engineering, Purdue University[a]
OPTLIB	A library of optimization programs	School of Mechanical Engineering, Purdue University[a]
BOX	Box's Complex method	
GS	Griffith-Stewart method	
OPTIVAR	A library of optimization programs	Prof. J. N. Siddall, Department of Mechanical Engineering, McMaster University, Hamilton, Ontario Canada L8S 4L7
ADRANS	Adaptive random search	
FLETCH	Fletcher's gradient search	
JO	Jacobson-Oksman method	
PDS	Powell's Conjugate direction search	
SEEK	Hooke and Jeeves Pattern Search	
VF02AD	Powell's successive quadratic programming method	Harwell Subroutine Library, United Kingdom Atomic Energy Authority Didcot, Oxfordshire England OX11 ORA

[a]Now available from: Prof. K. M. Ragsdell, Dept. of Mechanical and Aerospace Engineering, University of Missouri-Columbia, Columbia, MO.

Table 6. Results for pulping problem.

Objective function:	\$6436/hr
Variables:	
Cooking time fraction (hours)	0.643 (2.69)
Heating time fraction (hours)	0.240 (1.00)
Cooking temperature, °F	334
Active alkali charge, %	17.1
Sulfidity, %	20.0
Active alkali concentration in white liquor, lb/ft^3	5.80
Black liquor recycle split	0.290
Wood flow, lb/hr	368,000
Constraints:	
Pulp production	83,340
H-factor	2237
Furnace liquor concentration	0.6498
Downtime, hours	0.490
Heating + cooking time fractions	0.883
Heating time, hours	1.00
Liquor-to-wood ratio	3.50

and OPT were the most robust methods when used with the direct link interface. VF02AD was often successful, but care had to be taken to properly scale the problem.

The AI method was tested by developing linear and quadratic approximations of the test problem. The constraints were also cast into linear or quadratic form. A linear approximation for the process was developed by choosing selected values for the independent variables (in the allowed range) and obtaining converged solutions for that set of values. A resolution III, fractional factorial design was used to generate the values to be used for the independent variables. A linear regression program was then used to find the coefficients in the linear model. The quadratic approximation for the process was developed using a central composite experimental design. Linear regression was then used to develop the coefficients for the terms in the quadratic model.

The fraction of the complete range of the independent variable that is covered by the experimental design (and, therefore, the range of validity of the approximation) is a controllable parameter in the AI. If the full range is used, then one approximation defines the problem and, presumably, one solution will generate the optimum operating point. This is strictly true if the response surface is linear for the linear approximation and quadratic for the quadratic approximation. If the n-variable hypersurface is significantly curved, then the approximation is probably not good, and smaller ranges must be studied. Table 7 gives the number of complete simulations that must be executed to generate each approximation. Note that the GS method with the DLI takes fewer simulations to find a solution than the AI takes to generate a quadratic approximation. Obviously, if the AI is to be effective, then the linear approximation must be successful in two to four passes. Thus, initial ranges

Table 7. Comparison of the number of simulations required for direct-link optimization and for single sets of linear and quadratic approximations.

Problem	Number of Variables	Number of Simulations Required: For GS Direct Link Optimization	To Develop a Single Set of Quadratic Approximations[a]	To Develop a Single Set of Linear Approximations[a]
T2B	8	38	81	16

[a]Note that more than one set of approximations would be required during the optimization process.

must be chosen with care; successive passes with the approximation are centered on the optimum from the previous pass.

All optimization methods experienced problems with the AI. In general, these problems centered about trying to start from a nonfeasible solution and move to a feasible solution. In situations where the optimization method could find a solution, the number of simulations required was several times that required in the DLI.

CONCLUSION

Based on several realistic test problems, the best method of coupling an optimization package to a simulator is with a direct-link interface. This method of control is fairly easy to implement and allows a variety of optimization methods to be used. Linear and quadratic approximations to the problem are not a feasible method.

The most robust method seems to be the successive linear programming procedure developed by Griffith and Stewart. The reduced gradient method also gives very fast convergence, but can have problems. A viable technique is to use the

GS method to find the approximate hypervolume containing the minimum and then switch to the reduced gradient method for its excellent convergent properties.

The successive quadratic programming procedure as modifed by Powell and embodied in VF02AD is very fast and efficient when it works. Future work with this method may make it the procedure of choice.

The amount of computer time, as shown in Table 8, needed to find an optimal (or at least improved) operating point can be significant. Thus, such studies may be expensive in terms of personnel and computer time. However, a reduction in the capital cost of a new mill of only a fraction percent would give a return on investment of several thousand percent. Similarily, reduction of operating costs by pennies a ton can lead to large returns on investment.

Table 8. Direct link interfaces.

CPU Comparisons (Burroughs B6910):

Subproblem		GS	OPT	VF02AD
T2B	CPU time, min:sec	9:17	25:49	9:13
	CPU ratio	1.0	2.8	1.0

ACKNOWLEDGMENTS

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This paper is based on the doctoral dissertation of one of the authors (KES). The dissertation is on file at The Institute of Paper Chemistry and with University Microfilms.

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Use of a new pulp and paper system simulation-optimization program for kraft pulp mill optimization

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ABSTRACT

A versatile computer program capable of simulating and optimizing the steady-state operation of pulp and paper mills has been developed. Using the program, six variations of a kraft pulp mill optimization problem have been solved. An improved operating point was found for each case. The program can be used to assist in the design of new mills and for set point optimization in existing mills.

INTRODUCTION

General purpose, steady-state simulation programs such as GEMS (1), GEMCS (2), and MASSBAL (3) have been used throughout the pulp and paper industry for a variety of systems engineering applications (4,5,6,7). These simulators are used for improving the design of new mills and the operation of existing mills.

Another very powerful systems engineering tool is mathematical optimization. Optimization is the process of selecting the best of many alternatives. Many optimization techniques are available, but they have seen only limited use within the pulp and paper industry.

This paper describes a new systems engineering tool (OPPS) that combines optimization and general purpose, steady state simulation capabilities. A large scale application of the program abilities is presented: optimization of the operation of a kraft pulp mill.

PROGRAM DESCRIPTION

OPPS, Optimization of Pulp and Paper Systems, combines a steady state, modular simulator with two powerful optimization programs. The simulator is MAPPS, Modular Analysis of Pulp and Paper Systems, which is available through The Institute of Paper Chemistry. It contains a library of more than sixty modules representing operations in the pulp mill, paper mill, bleach plant, and steam-power system. The optimization programs employ a successive linearization-linear programming method (8) and a reduced gradient method (9). The two optimization methods were chosen after a thorough testing of many of the most popular constrained optimization methods. Either method can be used alone, or they can be used in a two stage procedure that provides greater reliability.

Any process that can be simulated with MAPPS can be optimized with OPPS. Users are free to define the measure of success, called an objective function, that is to be optimized. The user also specifies the MAPPS input variables that are to be used as independent variables in optimizing the objective function, and can enter any constraints on the system, such as a maximum equipment capacity or a minimum product quality. The optimization program determines a set of values for the independent variables, initiates a simulation using these values, and retrieves the appropriate information from MAPPS to calculate the objective function and constraint values. Many simulations may be required to find the optimum.

A strong emphasis was placed on making OPPS a reliable, easy to use, and easy to maintain program. Another important, yet secondary, goal was to make it efficient in its use of computer time. A full description of the development, structure, and use of OPPS is given in Ref. (10). A review of the optimization techniques and alternative methods for coupling the optimization package to the flowsheet simulator that were evaluated for use in OPPS is presented in Ref. (11).

KRAFT MILL OPTIMIZATION PROBLEM

A large scale kraft mill optimization problem was designed to show the power and usefulness of OPPS. Six versions of a basic problem have been optimized and are discussed here.

The problem involves improving the operation of a kraft pulping and recovery system, including a simple power plant and the C and E_1 stages of a CEDED bleachery. A simplified flow diagram for the system is given in Fig. 1.

The mill configuration and process specifications represent a hypothetical bleached kraft mill, not any one mill in particular. Twenty-eight equipment modules and 74 process flows with up to 35 components were used in the mill simulation. A more complete description of the system is given in Ref. (10).

[Fig. 1 here]

The heart of the simulation is a special digester model that incorporates pulping equations described in a separate article (12). These regression equations were developed from laboratory pulping data to give the relationships between the six independent variables: anthraquinone charge, effective alkali charge, sulfidity, liquor-to-wood ratio, cooking temperature, and H-factor, and each of five dependent variables: total yield, screened yield, kappa number, pulp viscosity, and residual effective alkali. This model is for a batch digester. Therefore, the results should be considered as averages over time.

Objective function

The objective of the optimization was to maximize an "operating profit" that was calculated by subtracting costs for wood, pulping and bleaching chemicals, fuel for the kiln and power boiler, and BOD removal, from credits for the production of bleached pulp, tall oil, and electricity. Prices, shown in Table I, were taken from published sources whenever possible. These sources are given in Ref. (10).

[Table I here]

Independent variables

In four versions of the problem, OPPS was given control of the nine MAPPS variables that are listed, together with their starting values and ranges, in

Table II. In two cases, anthraquinone was removed from the list. Variables 1 through 6 in Table II are called the pulping variables.

[Table II here]

Constraints

The principal constraints imposed on the optimization were:

1. The dilution factor was held at 3.0 to provide reasonably equivalent washing conditions in each case.
2. The concentration of the liquor from the concentrators was set at 63.0%.
3. A minimum unbleached pulp viscosity was set at 20 cp.
4. The viscosity was also constrained to be greater than the kappa number, since pulps with higher lignin contents presumably undergo a greater reduction in viscosity during bleaching.
5. The digester volume was held constant.
6. The final constraint reflected the use of the pulping regression equations in the digester model. It was used to prevent the optimization search from considering solutions in regions where the equations were not valid. The combined movement of the pulping variables was limited to the region covered by the experimental pulping data. The actual form of the constraint is discussed in Ref. (10).

The six constraints listed above were used in each of the six optimization cases. In addition, four of the cases described below had an additional constraint that represented a production bottleneck, and the MAPPS evaporator/concentrator model had an implicit capacity constraint - fixed heat transfer coefficients and areas. Other than the digester, evaporator and concentrator limitations and the special bottleneck constraints, no limitations were placed on the capacity of any equipment.

BASE case

A BASE case was used to tune the simulation and as a starting point and basis for comparison for the six optimization cases. The operating profit, independent variable values, and some important values from the simulation for the BASE case are presented in Table III. The values for variables 2 through 6 were taken from the center point of the experimental design used in the pulping experiments (12). The purpose of these experiments was to characterize the response of the kraft and kraft-anthraquinone pulping systems to changes in process variables under conditions which would result in low unbleached lignin contents. Consequently, the range (and therefore the center point) of effective alkali charge investigated was slightly higher than commercial practice. The anthraquinone charge was set to zero, and the remaining variable values were chosen to meet the dilution factor, concentrator liquor solids concentration, and digester volume constraints. Note that the viscosity is less than the kappa number at this starting point.

[Table III here]

Descriptions of the optimization cases

AQ and NO AQ cases

In the AQ case, the basic optimization problem described above was unchanged. In the NO AQ case, the anthraquinone charge was removed from the list of independent variables, and its value was set to zero.

PULP cases

Two PULP cases were optimized in which the amount of bleached pulp produced was limited to a maximum of 1006 o.d. ton per day, the BASE case production rate. This represents a paper machine or bleach plant bottleneck. The minimum pulp viscosity was raised from 20 cp in the PULP case to 30 cp in the PULP V > 30 case.

FURN cases

Two FURN cases were optimized with a constraint placed on the recovery furnace capacity. The amount of steam produced in the recovery boiler was limited to 524,000 lb/hr, which is the value from the BASE case. This represents a heat-release limitation on the furnace. The FURN-NO AQ case was run without the anthraquinone variable.

RESULTS AND DISCUSSION

The results from the six optimization runs and the base case simulation are presented in Table III. Table IV contains equipment capacity ratios for each case. These ratios were calculated by dividing the required capacity for a piece of equipment or a process by the corresponding base case capacity. The term capacity is defined as the flow rate of the important stream in a process, such as the wood flow in the wood handling section.

[Table IV here]

Following a discussion of some of the general trends in the results, each case is discussed separately. All references to costs refer to costs per ton of bleached pulp.

General discussion

In each of the six optimization cases, OPPS was able to find a set of operating conditions that resulted in a profit greater than that of the BASE CASE. The increases in the hourly operating profit ranged from 4.6% in the PULP V > 30 case to 28.8% in the AQ case. As one would expect, the most heavily constrained case, the PULP V > 30 case, had the smallest profit increase. The large increases of up to 28% in the equipment capacities required in the AQ and NO-AQ cases would exceed the available capacities in most mills. Therefore, the results from those two cases might not be considered practical from the point of view of improving current operating conditions. The smaller equipment capacity increases in the other four cases would be practical in many mills. The AQ and NO-AQ cases still serve several purposes, however. First, they provide a basis for comparison for the other cases that emphasize the severity of the FURN and PULP constraints. Second, they identify the areas where capital expenditures would be of greatest benefit. Finally, they show the potential danger in not thoroughly analyzing the results. Considering the results in Table III alone may lead one to conclude that by merely changing the nine independent variables the operating profit may be increased by over $2000 per hour, when, in fact, large increases in equipment capacities are also required.

In each case the experimental design constraint was active at the solution, which meant that the optimization program could not move any pulping variable further from its starting point value unless it moved another one closer to its starting value. Thus the program not only had to determine in which direction to move each variable to improve the hourly profit and to satisfy the constraints, but it also had to determine the relative importance of changing one variable instead of another. The fact that the total combined movement of the six pulping variables was limited should be kept in mind in viewing the results.

Another general observation is that the optimization program first increased the production rate and then tried to increase the profit per ton of pulp, compared to the BASE case. In the three trials where the production increased by 10% or more, the NO AQ, AQ, and FURN cases, the profit per ton of pulp was increased by $7 or less. However, in the three trials where the production rate could not be significantly increased, the per ton profits were raised by $14 to $24.

Not surprisingly, the effective alkali charge was significantly lower in each case than the base case value of 18%. There are several reasons for this trend. Lower effective alkali charges increase the pulping yield, which in turn increases the production rate. Direct and indirect cost reductions are achieved through reduced requirements for pulping chemicals, lime, and kiln fuel, and by lower evaporator steam demands and lower heat losses with the smelt. A decrease in the effective alkali increases the pulp viscosity, which is important in cases in which the minimum viscosity constraint is active.

The final general observation is that the liquor-to-wood ratio in each solution is less than the starting value of 4.0. One possible reason for this is that the reduced liquor level allows more wood to be cooked in the fixed volume digester. A liquor-to-wood ratio of 3.5 allows about 9% more wood, and a 3.0 ratio allows about 20% more wood to be put into the digester. This results in a production rate increase. This effect may not be realistic, since below a certain liquor-to-wood ratio the wood charge is limited by the chip packing density, not the liquor-to-wood ratio. Of course, the impact that the liquor-to-wood ratio has on the yield, kappa number, and pulp viscosity may also be important in any particular case. It should be noted that the values in Table III are actually water-to-wood ratios, which closely approximate volumetric liquor-to-wood ratios.

NO AQ case

The hourly profit of $13,300 for the NO AQ case solution from Table III represents a $2,800 increase over the BASE case profit. Most of this increase came from a 24% production rate increase, although the profit per ton of pulp was also slightly higher. Reductions in the cooking time and liquor-to-wood ratio and an increase in the yield contributed to the production increase. Note that the 65 psia evaporator steam pressure indicates that the evaporators were operating at full capacity, which put a limit on the production rate increase.

AQ case

The results for the AQ case are similar to those of the NO AQ case. The $220 hourly profit increase over the NO AQ case was due to a higher production rate, since the per ton profit level was lower. An anthraquinone charge of 0.06% led to a yield increase and cooking time decrease that caused the small but significant production increase.

PULP case

With the production rate fixed in the PULP trial, OPPS could increase the hourly profit only by increasing the profit per ton of pulp. It was able to raise the profit to $274 per ton and the hourly profit to $11,470. Three major cost reductions were achieved: A \$5 decrease in both the caustic and bleaching chemical costs, and a drop of \$13 in the power boiler fuel cost. The high sulfidity-low effective alkali combination required no caustic makeup. The low kappa number was responsible for the decrease in bleaching chemicals usage. Several things contributed to the lower fuel cost. First, the low liquor-to-wood ratio and cooking temperature reduced the digester steam demand. Second, the low yield-low kappa number combination resulted in more organics being burned in the recovery boiler, which increased its steam output and decreased the amount required from the power boiler. The largest equipment capacity increase was 4% in the recovery boiler.

PULP V > 30

As the results in Table III indicate, the increase in the minimum viscosity level severely affected this case. The hourly profit was decreased by \$490 compared to the PULP case. Significantly lower temperature and H-factor values were primarily responsible for the viscosity increase. Most of the profit decrease was caused by higher bleaching and power boiler fuel costs, which, in turn, were caused by the higher yield and kappa number. The CE bleaching cost is proportional to the kappa number. The yield and kappa number increases reduced the amount of organics burned in the recovery furnace, and therefore reduced the steam production from that unit. Since the recovery boiler produces five to ten times as much steam as the power boiler, even a small decrease in the recovery boiler steam production requires a relatively large increase in the power boiler's production. All of the base case equipment capacities were sufficient for this solution.

FURN case

Anthraquinone played an important role in this recovery boiler-limited case. A charge of 0.12% created a high yield, low kappa pulp, which allowed a 10% pulp production increase with no change in the recovery boiler capacity. The high yield, low kappa pulp produced a much lower than normal ratio of the amount of carbohydrates dissolved to the amount of pulp produced, which allowed more pulp to be produced at the same recovery boiler steam production rate. Decreases in wood, bleaching chemicals, and kiln fuel costs more than offset the anthraquinone cost of $10.8. The power boiler and brownstock washing capacity requirements increased by about 10% and 8%, respectively.

FURN-NO AQ

With no anthraquinone available in this recovery boiler-limited case, OPPS could only increase the production by 4%. However, it was able to increase the profit per ton by $10 over the FURN case. The major cost difference between these two cases was the $10.8 anthraquinone cost in the FURN case. The largest equipment capacity increase was 3% in the brownstock washers.

CPU time requirements

OPPS used from 9 to 37 minutes of processor time on a Burroughs B6900 computer to solve each of these problems. The amount of time required to solve a given problem depends on the number of independent variables, on the speed of convergence of the simulation, and on the generally unpredictable difficulty in solving the problem. Although relatively large amounts of CPU time may be required for combined simulation and optimization studies, the costs in most applications will be small compared to the benefits derived from the optimization of an entire process or mill.

Limitations

Three things can limit the usefulness of the OPPS results. First, the MAPPS process models must correctly model the process under consideration. Second, the process specifications used in the base case simulation must accurately reflect the operating conditions of the mill. Finally, the optimization problem must be properly defined to include the appropriate objective function, independent variables, and constraints. There are never any substitutes for a carefully designed problem and a thorough analysis of the results.

CONCLUSIONS

OPPS is an advanced systems engineering tool for the pulp and paper industry. It has the potential to be extremely useful for applications in research, management, and production. We have demonstrated its usefulness by optimizing the operations of a hypothetical kraft pulp mill under several production bottlenecks. For example, we have found that anthraquinone could be used to increase the production rate and profit when the mill was recovery boiler limited but not when it was pulp production limited.

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I. Assumed costs used in profit calculation

Item	Unit	Price/Unit
Wood	o.d. lb	$0.025
Anthraquinone	lb	2.00
Caustic	lb	0.16
Saltcake	lb	0.04
Chlorine	lb	0.72
Lime	lb	0.029
Fuel oil	lb	0.125
BOD treatment	lb removed	0.289
Bleached slush pulp	o.d. ton	400.00
Tall oil	lb	0.10
Electricity	kwh	0.03

III. Results from the base case and the six optimization cases

Hourly Operating Profit	BASE CASE $10,500	NO AQ $13,300	AQ $13,520	PULP $11,470	PULP V > 30 $10,980	FURN $11,770	FURN NO AQ $11,460
Anthraquinone	0.00	0.00	0.06%	0.00	0.00	0.12%	0.00
Effective alkali	18.0%	14.6%	14.4%	15.6%	15.9%	15.5%	15.4%
Sulfidity	25.0%	28.0%	25.4%	31.7%	34.0%	27.4%	33.8%
Liquor-to-wood ratio	4.00	3.69	3.74	2.90	3.15	3.02	3.07
Cooking temp.	343°F	354°F	354°F	339°F	328°F	330°F	331°F
H-factor	2000	2480	2320	2670	1560	1570	1690
Wood flow, lb/hr	389,000	472,000	478,000	395,000	381,000	404,000	395,000
Wash flow, lb/hr	764,000	948,000	971,000	753,000	763,000	839,000	790,000
Evap. stm press, psia	49.5	65.0	65.0	51.5	49.5	56.4	53.0
Production, tpd	1006	1244	1279	1006	1006	1112	1042
Cooking yield	45.2	46.3	46.8	44.1	46.1	48.0	46.1
Bleaching yield	95.4	95.1	95.4	96.7	95.5	96.0	95.6
Cooking time, hours	1.54	1.12	1.04	2.52	2.41	2.30	2.34
Kappa number	25.6	27.3	25.3	18.3	25.0	22.3	24.5
Viscosity,	24.8	29.3	27.5	19.9	30.0	27.1	29.2
Operating Profit per ton of pulp	$250	$257	$254	$274	$262	$254	$264
COSTS in dollars per ton of pulp produced:							
Wood	116	114	112	118	114	109	114
Anthraquinone	0	0	5.42	0.06	0	10.8	0
NaOH, pulping	4.91	3.82	4.50	0	0	2.28	0
Na_2SO_4	3.87	3.42	2.89	5.56	5.61	4.16	5.50
Bleaching chemicals	18.8	20.0	18.5	13.2	18.4	16.3	18.0
Lime	0.98	0.77	0.76	0.82	0.79	0.78	0.78
Fuel, kiln	17.7	13.9	13.6	14.9	14.4	14.0	14.1
Fuel, power boiler	19.5	18.5	19.6	6.87	15.9	19.0	14.9
BOD removal	5.27	5.65	5.18	3.58	5.13	4.50	5.00
CREDITS in dollars per ton of pulp produced:							
Pulp	400	400	400	400	400	400	400
Tall oil	13.3	13.0	12.8	13.4	13.0	12.4	13.0
Electricity	24.3	23.6	23.4	22.8	22.9	22.2	22.8
CPU time, minutes	--	30.7	35.9	35.9	8.9	32.5	28.5

IV. Equipment capacity ratios: Equipment capacity relative to the BASE case capacity

	BASE CASE	NO AQ	AQ	PULP	PULP V > 30	FURN	FURN NO AQ
Wood handling	1.00	1.20	1.23	1.02	0.98	1.04	1.02
Digester	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Brownstock washers	1.00	1.24	1.27	0.99	1.00	1.10	1.03
Black liquor operations	1.00	1.11	1.10	1.01	0.99	1.04	1.02
Recovery boiler	1.00	1.22	1.22	1.04	0.96	1.00	1.00
Power boiler	1.00	1.17	1.28	0.35	0.82	1.08	0.79
Turbine	1.00	1.21	1.23	0.94	0.94	1.01	0.97
Lime kiln	1.00	0.97	0.98	0.84	0.81	0.88	0.82

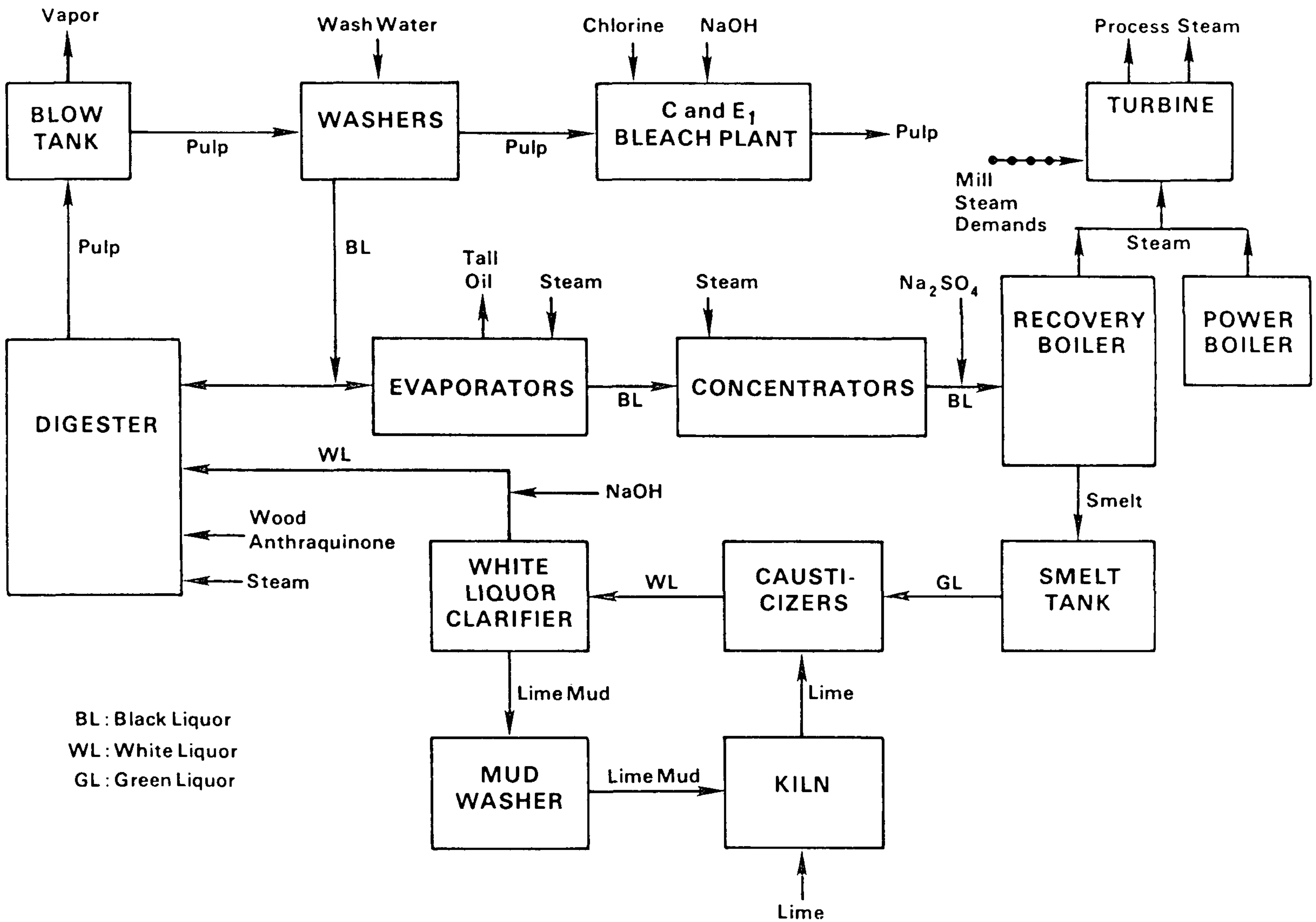

Figure 1. Simplified flow diagram of the hypothetical kraft pulp mill.